BEYOND MONTE CARLO — STATISTICAL VERIFICATION AND VALIDATION OF SPACE SYSTEMS

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Final Report

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A. OBJECTIVES

Our objective was to develop computationally efficient techniques that go beyond the traditional Monte Carlo (MC) methods of uncertainty analysis in dynamical systems. A considerable body of existing work [1] is directed to using MC methods to obtain the expected value of some function. However, in order to understand the totality of system behavior under non-linear dynamics and non-Gaussian initial probability distribution functions (PDFs), it is useful to evolve the entire PDF of the state and not just try to estimate an expected value and variance. Several statistical analyses can be achieved using moments (mean, variance). For Gaussian distributions, these two quantities are enough to determine the PDF. But the PDF evolution under uncertainty and nonlinear dynamics may not remain Gaussian and higher moments will be needed to approximate the PDF. Accuracy in computation of a given order moment requires exponential increase in the number of sample points required in MC simulations. Thus, our objective was to directly estimate the PDF in a computationally efficient manner. Specifically, we would develop a transfer operation method [2] to evolve the PDF of a dynamical system. Achieving this objective would provide an alternative to Monte Carlo methods to verify and validate future space systems. Our focus was on a demonstration within the entry, descent, and landing (EDL) domain, as that is the one of the more critical phases of a mission, and also represents a computationally intensive use of MC simulation methods.

B. APPROACH AND RESULTS

We illustrate PDF evolution for a particularly simple dynamical system in Figure 1. A stable one-dimensional linear system: $dy/dt = -a\, y$, has initial states 'y' that are expected to go to the origin with a speed proportional to the magnitude of the parameter 'a'. Our simple example has the initial state 'y' Gaussian distributed with mean of 3 and standard deviation of 1, and the parameter 'a' uniformly distributed in the interval [0.4, 1]. Figure 1(a) shows the PDF at t=0 and Figure 1(b) shows the distribution at t=2. In Figure 1(b), the states for those systems with higher values of 'a', and consequently faster dynamics, get to the origin quicker than those with lower values of 'a'. The skewed shape of the distribution in Figure 1(b) reflects this difference in behavior over the range of 'a'. We now discuss various approaches to determining this PDF evolution for a complex dynamical system. The limitations of MC-based dispersion analysis are well known; i.e., poor computational scalability and lack of a methodology to quantify the evolution of uncertainty in a statistically consistent manner. Consequently, researchers have pursued different methods for uncertainty propagation in dynamical systems. The methods may be grouped in two broad categories: parametric (where one evolves the statistical moments) and non-parametric (where one evolves the full PDF).

There have been three major directions in parametric propagation of uncertainty:

- The simplest method in this category assumes a linear state space description of the form dx/dt = A x. With the initial condition uncertainty assumed to be Gaussian, one then propagates the mean and covariance matrix by the well-known state and Riccatti equations. The major drawback is that a typical EDL system with large number of states involving highly nonlinear dynamics and non-Gaussian initial joint PDF does not fit in this framework.

- In polynomial chaos (PC) method, one derives a set of deterministic ordinary differential equations (ODEs) using either Galerkin projection or stochastic collocation and then solves the resulting set of ODEs. Although this method can handle nonlinear dynamics with non-Gaussian uncertainties, one ends up solving a higher-dimensional state-space problem, which becomes intractable for a realistic EDL simulation. Further, the method is difficult to apply for large nonlinearities and the computational performance degrades (due to finite-dimensional approximation of the probability space) if long-term statistics are desired. A recent attempt to apply this method in EDL domain can be found in [3].

- Another method in this category is called the direct quadrature method of moments, where the PDF is approximated as a sum of Dirac delta functions with evolving parameters. This method has a problem of meeting various closure conditions on the resulting moments.

Non-parametric propagation of uncertainties can be performed using either an approximate method or a direct method.

- In the approximate method, one tries to estimate (in non-parametric sense) the underlying PDF. The method aims to approximate the solution of the PDF transport equation. This method is widely exercised in statistics community [4] under the name of kernel density estimation, although most applications there a concerned with static data. In a dynamical system, one must do a dynamic optimization to determine the optimal values of the parameters at every time instant. The method can suffer from high computational cost arising due to the explicit enforcement of normality constraint and moment closure constraint at each step of dynamic optimization procedure. Moreover, for high-dimensional state spaces like planetary EDL, recursively performing constrained optimization becomes challenging.

- In the direct method, one works to directly solve the PDF transport equation and as opposed to approximating its solution. If the dynamics are assumed to be deterministic, this transport equation reduces to the stochastic Liouville equation (SLE) [5], which is a quasi-linear partial differential equation (PDE), first order in both space and time. The SLE is an example of the Perron-Frobenius (PF) operator [2] method of propagating the PDF evolution. The evolution of the PDF is given by the action of the PF operator P_t on the density f(y); i.e., $u(t,y) = P_t f(y)$, which in turn satisfies the partial differential equation $\partial u/\partial t + \sum \partial(uF_i)/\partial y_i = 0$, where F represents the dynamics of the system and the summation is over all the state components. The SLE can be easily solved in a direct way using the method of characteristics (MOC). Since all the statistics can be derived from the PDF, from an information point of view, it is definitely superior to the parametric propagation methods. In the SLE method, instead of individual realizations (initial conditions and/or parameters), one propagates the ensemble of realizations. This, in essence, means that the number density of trajectories meets the continuum hypothesis [5]. Since the SLE is solved directly, the solutions will satisfy the criteria to be a PDF, and hence the problems like moment closure or normality constraints are not required to be explicitly enforced.

We had originally considered also analyzing solution methods for dynamical systems under conditions of stochastic forcing; i.e., solving transport equations using the Fokker-Plank-Kolmogorov (FPK) formulation [6]. However, we have since chosen to focus on solving the PF operator-derived SLE equations. This allowed us to give a more in-depth treatment to the SLE techniques for PF solutions and defer the FP formulation to a later effort.

Milestone. PF Solver Implementation — We developed PF solvers based upon solving the SLE equation in two different implementations utilizing Matlab and C++ codes for systems specified by analytical equations for the system dynamics. In this case, the gradient terms needed for the SLE solution can be obtained analytically. This was applied to the EDL problem to solve the so-called Vinh's equations [7]. We used the evolved PDFs to compute the marginal distributions that correspond to those typically used in EDL analysis. The results of using this solver and the corresponding MC results are shown in Figure 2 for the case of the longitudinal Vinh's equations with three states, height (h), velocity (V) and flight-path angle (FPA) solved for 5000 initial conditions. On the left, the red (solid) uni-variate curve corresponds to PF and the blue (dash-dot) lines to MC. The MC and PF uni-variate densities are in good match. To the right are the bi-variate marginal distributions, with the top row in the bi-variate plots corresponding to MC and the bottom one to PF solutions, respectively. The bi-variate marginals show the general trend that PF-derived marginals capture the concentration of probability mass well (by virtue of the probability weights obtained by solving SLE), while the MC results tend to smear it out (because of bin-counting). This can be seen, for example, in FPA vs. V bi-variate plots.

Milestones. Scaling Software for handling large number of states; Code module testing at JPL for example EDL application — For systems with a large number of states (e.g., systems with attitude dynamics or multiple bodies), we added a PF solver using the MOC to the DSENDS simulation system at JPL. DSENDS uses a computationally efficient multibody dynamics engine with dynamics computation scaling linearly with the degree of freedom. Our initial implementation uses a numerical differencing method to compute the gradient terms needed for the SLE solver. We then applied this newly extended DSENDS system to a realistic example involving the Mars Pathfinder spacecraft together with high-fidelity atmospheric and nonlinear aerodynamics models. We show some of the numerical results from these simulations. The graph on the left in Figure 3 shows the evolution of the probability weights for a system with both translational and attitude dynamics within a single solution (a 12-state system) obtained by the MOC. It can be seen that, in the initial portion of the trajectory, the weight peaks as the system slows down and the trajectories crowd into a smaller region of the velocity space. However, towards the latter part of the trajectory, the weight starts to decrease to reflect the dispersion produced by the attitude instability in that portion of the flight regime. The plot on the right in Figure 3 shows the evolution of solutions obtained by the MOC for an ensemble of trajectories. The multidimensional state has been projected into relative-flight-path (rfpa) and atmosphere-relative velocity magnitude (rmag) coordinates. The individual solutions are color-coded with their end-of-trajectory probability weights, with a rainbow color coding in which violet-blue reflect lower values and orange-red reflect larger values.

Milestone: Benchmarking performance and verification — A specific quantitative objective was to determine the PDF of the system state for systems with dozens of states with parametric uncertainty in 100s of parameters using 2 orders of magnitude (i.e., 100×) less computation than the traditional Monte Carlo methods. We had shown this computational advantage for simple systems with benchmarking results in the initial proposal. However, during the performance of the DRDF task, we came to the realization that this benchmarking was more difficult than we had anticipated for the more complex systems. The PDF solution using the MOC gives the exact probability weight for the evolved state PDF for a particular point in the space with far less computation than an MC histogram method of estimating the PDF around that point. However, in most EDL analysis, the MC method is not used to directly obtain PDF values but is used instead to obtain estimates of various conditional distributions of the state — e.g., distribution of the landing footprint; i.e., P(x,y|z=0). Obtaining these conditional distributions from a PDF requires evaluating the associated marginal distributions for the evolved PDF, which in turn are obtained as integrals over the PDF. Note that when computing integrals (i.e., expectations), whether one uses the evolved state with its distribution (obtained by the solving SLE using the MOC) or the initial distribution, in the limit where a large number of points are sampled, the results are mathematically equivalent. One therefore has to compare the computational cost of obtaining the marginal distribution from the evolved PDF using a limited set of sample points to those obtained by MC estimates obtained by histograms generated from the initial PDF distributions. An additional factor that has to be resolved in the benchmarking process is to hold the desired accuracy level for each method to be the same. We are currently performing computational experiments using the low-dimensional forms of the analytical Vinh's equations to address these questions.

Specifically, we are:

- Using the Kullback Liebler (KL) measure to determine how close the numerically obtained distributions are to the truth distribution (where computable analytically).

- Investigating integration methods in the high-dimensional spaces to obtain the "area" under the evolved PDFs, and techniques such as adaptive refinement to ensure that the evolved PDF values are obtained over the region of interest.

- Determining cases where it may be advantageous to obtain conditional distributions using the evolved PDF instead of traditional MC estimation of the integrals.

C. SIGNIFICANCE OF RESULTS

The techniques we have demonstrated to date give us an exact method to obtain the PDF as evolved through a dynamical system. Using the PF method, if one knows the functional form of the initial PDF, one could generate any desired number of samples of that PDF using Markov Chain Monte Carlo (MCMC) and then propagate the PDF for these “high-initial-probability" samples. The samples would be assigned weights (value of the joint PDF) at later instants of time by solving the Liouville equation using the method of characteristics. Since the exact probability weights are calculated in PF method, one no longer needs huge number of samples to approximate the PDF. On the contrary, in the MC method, approximate joint PDF construction at a given time instant requires binning and counting samples in a large number of histogram bins.

The temporal evolution of the PDF gives the EDL analyst additional insight into the behavior of the system under uncertainty. Especially in the case of low-dimensional EDL systems, the numerical results appear to be more precise when compared to some of the “smeared out” MC results. An initial implementation of MOC solution methodology is now available in the DSENDS simulator system and allows for high-fidelity numerical experiments.

For statistical analyses, which are based on expectation and variance, the PF approach may not provide a significant advantage over MC in terms of accuracy and computational time. As discussed earlier, for higher-dimensional systems where conditional distributions (using expectations) needs to be determined, the direct advantage of the PF methodology has not yet been established. Nevertheless, we are currently evaluating if the PF solutions can be used in conjunction with other MC methods such as importance sampling or MCMC, where various sampler and proposal densities need to be determined and could be obtained from the PF solutions. However, for analyses where the PDF is required, PF will outperform MC. Examples of such analyses include state and parameter estimation, robust and optimal control with probabilistic uncertainty, and system reliability analysis where system-level uncertainty is determined based on component-level uncertainty.

D. NEW TECHNOLOGY

The emphasis here has been on algorithmic exploration of uncertainty propagation in dynamical systems. The implementation of the MOC method for evolving the PDF represents a new software technology now available as an initial implementation in the DSENDS systems. After further validation and refinement, this will be reported as a new software technology.

E. FINANCIAL STATUS

The total funding for this task was $200,000, all of which has been expended.

F. ACKNOWLEDGEMENTS

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G. PUBLICATIONS AND PRESENTATIONS

[A] Abhishek Halder and Raktim Bhattacharya, “Beyond Monte Carlo: A Computational Framework for Uncertainty Propagation in Planetary Entry, Descent and Landing,” submitted to *AIAA GNC Conference,* Toronto, Canada, 2010.

H. REFERENCES

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I. FIGURES

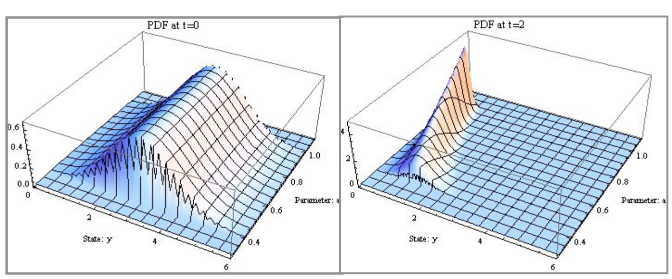

Figure 1. Example of PDF evolution for a simple linear system.

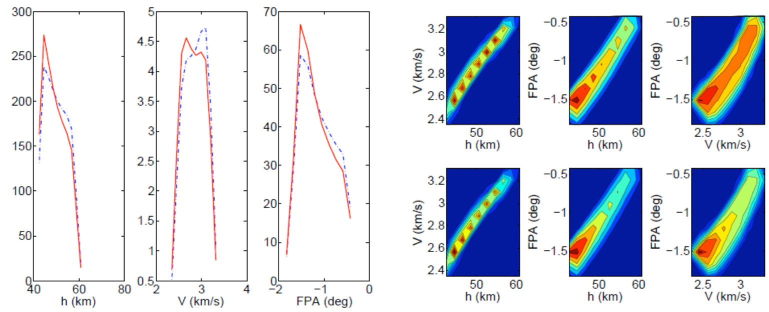

Figure 2. Solutions obtained by both MC and PF methods.

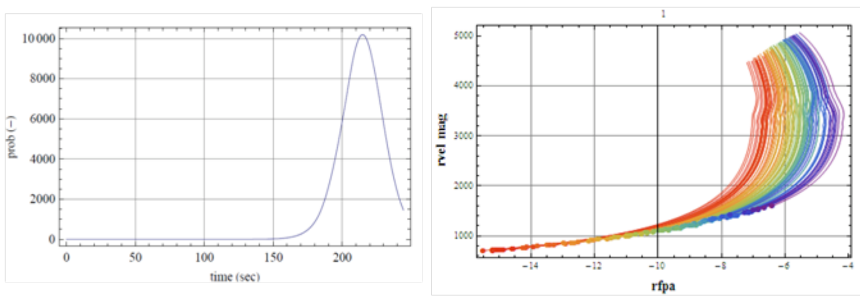

Figure 3. Evolution of PDF weights and ensemble of solutions.